

Phosphonothioic acid, methyl-, O,o-diethyl ester

6996-81-2 | DTXSID10220237

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

## Model Results

**Predicted value:** 8.61e-03 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 5.48e-01

**Confidence level:** 7.54e-01

## Nearest Neighbors from the Training Set

Image not found

tert-Butyl methacrylate

**Measured:** 7.03e-03

**Predicted:** 8.19e-03

Image not found

Butyl methacrylate

**Measured:** 5.63e-03

**Predicted:** 7.93e-03

Image not found

Benzyl acetate

**Measured:** 2.06e-02

**Predicted:** 1.22e-01

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Ethyl benzoate

**Measured:** 4.79e-03

**Predicted:** 9.44e-02